=> b reg
FILE 'REGISTRY' ENTERED AT 14:34:09 ON 11 JAN 2011

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DICTIONARY FILE UPDATES: 10 JAN 2011 HIGHEST RN 1258930-61-8

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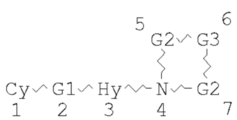
=> d que sta l14
L5   STR



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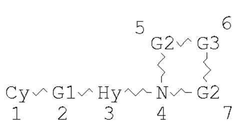
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E2 N AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   7

STEREO ATTRIBUTES: NONE
L6   1749673 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 46.195/RID AND
                NRS>=3
L14   26410 SEA FILE=REGISTRY SUB=L6 SSS FUL L5

100.0% PROCESSED 1749673 ITERATIONS   26410 ANSWERS
SEARCH TIME: 00.00.12

=> d que sta l18
L5   STR



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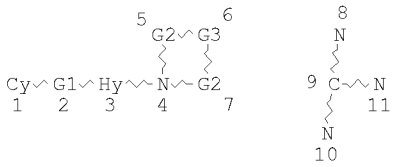
REP G2=(1-3) C
VAR G3=C/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E2 N AT   3

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
L6 1749673 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 46.195/RID AND NRS>=3
L14 26410 SEA FILE=REGISTRY SUB=L6 SSS FUL L5
L16 STR



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REP G2=(1-3) C
VAR G3=C/N
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E2 N AT 3

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STEREO ATTRIBUTES: NONE
L18 16 SEA FILE=REGISTRY SUB=L14 SSS FUL L16

100.0% PROCESSED 18 ITERATIONS 16 ANSWERS
SEARCH TIME: 00.00.01

=> b zcap

FILE 'ZCAPLUS' ENTERED AT 14:34:28 ON 11 JAN 2011
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 11 Jan 2011 VOL 154 ISS 3
FILE LAST UPDATED: 10 Jan 2011 (20110110/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2010

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the fourth quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

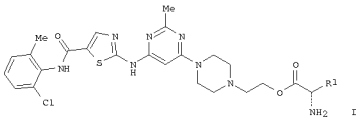
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d bib abs hitstr l22 tot

L22 ANSWER 1 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN
AN 2009:1556443 ZCAPLUS
DN 152:97483
TI Preparation of Dasatinib derivatives as antitumor agents
IN Wang, Jianmin
PA Beijing Laibo Sailusen Pharmaceutical Science and Technology Co., Ltd., Peop. Rep. China
SO Faming Zhuanli Shenqing Gongkai Shuomingshu, 25pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI CN---101597284	A	20091209	2009CN-010089059	20090722
PRAI 2009CN-010089059		20090722		

OS CASREACT 152:97483; MARPAT 152:97483
GI



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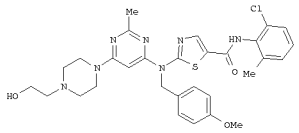


II

AB Title compds. [I; wherein R1 = H, (un)substituted alkyl, cycloalkyl, or aryl, etc.], and their pharmaceutically acceptable salts thereof, were prepared as antitumor agents. Thus, the invention compound I (R1 = i-Bu) was prepared by esterification of compound II (prepared given) with Boc-L-leucine followed by deprotection.
IT **1094075-80-5P** **1203456-85-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of Dasatinib derivs. as antitumor agents)
RN 1094075-80-5 ZCAPLUS
CN L-Arginine, 2-[4-[6-[[5-[[(2-chloro-6-methylphenyl)amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazinyl]ethyl ester (CA INDEX NAME)

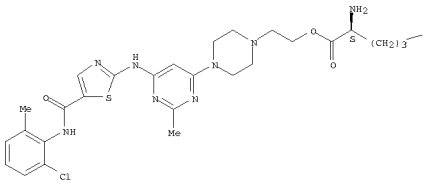
Absolute stereochemistry.

L22 ANSWER 1 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)

PAGE 1-B

L22 ANSWER 1 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)

PAGE 1-A

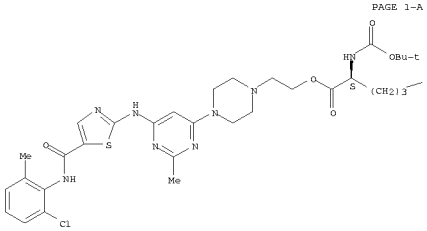


PAGE 1-B

RN 1203456-85-2 ZCAPLUS
CN L-Arginine, N2-[(1,1-dimethylethoxy)carbonyl]-, 2-[4-[6-[[5-[[(2-chloro-6-methylphenyl)amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazinyl]ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

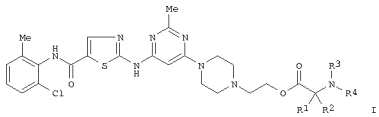
PAGE 1-A



L22 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN
AN 2008:1467949 ZCAPLUS
DN 150:77944
TI Preparation of Dasatinib amino acid derivatives as antitumor agents
IN Wang, Jianmin
PA Peop. Rep. China
SO Faming Zhuanli Shenqing, 45pp.
CODEN: CNXXEV
DT Patent
LA Chinese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI CN---101334600	A	20081203	2008CN-010111853	20080516
CN---100532381	C	20090826		
PRAI 2008CN-010111853		20080516		

OS CASREACT 150:77944; MARPAT 150:77944
GI



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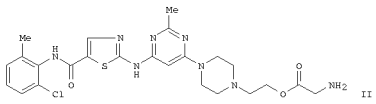


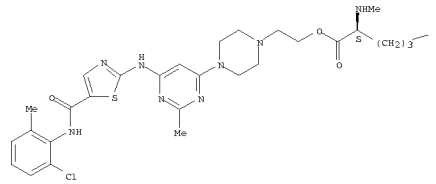
II

AB The title Dasatinib amino acid derivs. I [wherein R1-R4 = independently H, (un)substituted (cyclo)alkyl, aryl, or aralkyl; or R1 and R2 form an (un)substituted cycloalkyl; or R2/R3 or R3/R4 form an (un)substituted heterocyclyl; with the proviso R2(R1) ≠ iso-Pr when R1(R2), R3, and R4 = H], or pharmaceutically acceptable salts, solvates, polycrystals, enantiomers, or racemic mixts. thereof were prepared for treating tumor, such as leukemia, myelodysplasia, Hodgkin's disease, non-Hodgkin's lymphoma, etc. For example, II was prepared from reaction of Dasatinib with N-BOC-glycine followed by removing the BOC group. In biol. test, II showed 41% bioavailability. The compds. can be used as prodrugs of Dasatinib, producing Dasatinib by enzymic hydrolysis.
IT **1094074-82-4P** **1094074-83-5P** **1094074-85-7P**
1094074-86-8P **1094075-80-5P** **1094075-81-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of Dasatinib amino acid derivs. as antitumor agents)
RN 1094074-82-4 ZCAPLUS
CN L-Arginine, N2-methyl-, 2-[4-[6-[[5-[[(2-chloro-6-methylphenyl)amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazinyl]ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

L22 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)

PAGE 1-A

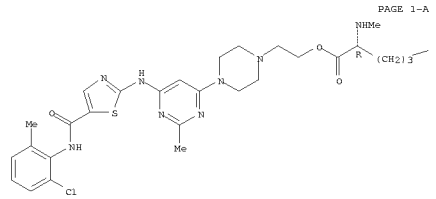


PAGE 1-B

RN 1094074-83-5 ZCAPLUS
CN D-Arginine, N2-methyl-, 2-[4-[6-[[5-[[(2-chloro-6-methylphenyl)amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazinyl]ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

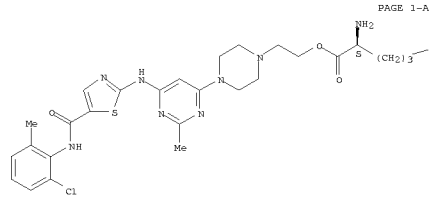
L22 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)

PAGE 1-B

RN 1094075-80-5 ZCAPLUS
CN L-Arginine, 2-[4-[6-[[5-[[(2-chloro-6-methylphenyl)amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazinyl]ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

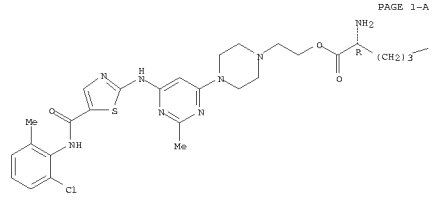


PAGE 1-B

RN 1094075-81-6 ZCAPLUS
CN D-Arginine, 2-[4-[6-[[5-[[(2-chloro-6-methylphenyl)amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazinyl]ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

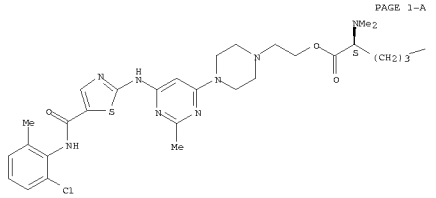


L22 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)

RN 1094074-85-7 ZCAPLUS
CN L-Arginine, N2,N2-dimethyl-, 2-[4-[6-[[5-[[(2-chloro-6-methylphenyl)amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazinyl]ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

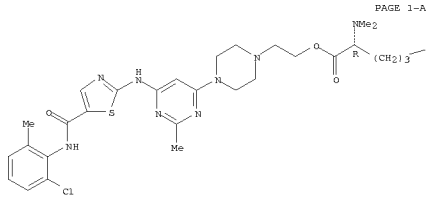


PAGE 1-B

RN 1094074-86-8 ZCAPLUS
CN D-Arginine, N2,N2-dimethyl-, 2-[4-[6-[[5-[[(2-chloro-6-methylphenyl)amino]carbonyl]-2-thiazolyl]amino]-2-methyl-4-pyrimidinyl]-1-piperazinyl]ethyl ester (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



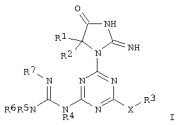
L22 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)

PAGE 1-B

L22 ANSWER 3 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN
AN 2008:729540 ZCAPLUS
DN 149:54023
TI Preparation of novel imidazolones as guanylyl cyclase receptor A (GC-A) agonists
IN Namikawa, Koji; Shimamoto, Tetsuo; Kitano, Katsuhiko; Koyama, Yoshiaki
PA Asubio Pharma Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 34pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP--2008137897	A	20080619	2006JP-000322504	20061129
PRAI 2006JP-000322504		20061129		

OS MARPAT 149:54023
GI



I

AB Title compds. I (R1, R2, R4-R7 = C1-6 alkyl, C6-14 aromatic hydrocarbyl, H; R3 = C1-10 alkyl, C6-14 aromatic hydrocarbyl, H; X = NH, O), their salts, or their solvates are prepared The imidazolones show diuretic activity, thus useful for treatment of acute heart failure. Thus, 350 mg N-(4-anilino-6-chloro-1,3,5-triazin-2-yl)-L-leucine Me ester was treated with 300 mg guanidine at 100° in propionitrile, then treated with aqueous CF3CO2H to give 348 mg 1-[4-(2-amino-5-isobutyl-4-oxo-4,5-dihydro-1H-imidazol-1-yl)-6-anilino-1,3,5-triazin-2-yl]guanidine ditrifluoroacetate, which showed GC-A receptor agonist activity with ED50 value of 4000 nM in CHO/human GCA (4A) cells.

IT **1033127-69-3P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of (imidazolyltriazinyl)guanidines as guanylyl cyclase receptor A agonists for treatment of acute heart failure)

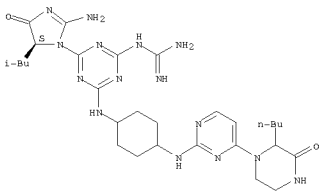
RN 1033127-69-3 ZCAPLUS
CN Guanidine, N-[4-[(5S)-2-amino-4,5-dihydro-5-(2-methylpropyl)-4-oxo-1H-imidazol-1-yl]-6-[[4-[[4-(2-butyl-3-oxo-1-piperazinyl)-6-chloro-2-pyrimidinyl]amino]cyclohexyl]amino]-1,3,5-triazin-2-yl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 1033127-68-2
CMF C29 H44 Cl N15 O2

Absolute stereochemistry.

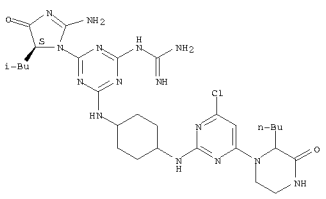
L22 ANSWER 3 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L22 ANSWER 3 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT **1033127-71-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (imidazolyltriazinyl)guanidines as guanylyl cyclase receptor A agonists for treatment of acute heart failure)

RN 1033127-71-7 ZCAPLUS
CN Guanidine, N-[4-[(5S)-2-amino-4,5-dihydro-5-(2-methylpropyl)-4-oxo-1H-imidazol-1-yl]-6-[[4-[[4-(2-butyl-3-oxo-1-piperazinyl)-2-pyrimidinyl]amino]cyclohexyl]amino]-1,3,5-triazin-2-yl]-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

CRN 1033127-70-6
CMF C29 H45 N15 O2

Absolute stereochemistry.

L22 ANSWER 4 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN
AN 2006:887712 ZCAPLUS
DN 145:293089
TI Preparation of 2-aminopyrimidine compounds as CXCR4 antagonists
IN Ochiai, Hiroshi; Onhata, Akira; Takaoka, Yoshikazu; Shibayama, Shiro
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 179pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO--2006090853	A1	20060831	2006WO-JP0303477	20060224
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP-----1852432	A1	20071107	2006EP-000714616	20060224
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
US-20090233908	A1	20090917	2007US-000816940	20070823
PRAI 2005JP-000050098	A	20050225		
2006WO-JP0303477	W	20060224		

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OS MARPAT 145:293089
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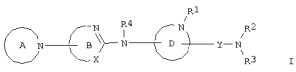

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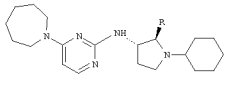


II

AB Title compds. I [ring A = (un)substituted heterocycle containing nitrogen; ring B = optionally substituted unsatd. heterocycle containing nitrogen; ring D = (un)substituted heterocycle containing nitrogen; X = nitrogen, carbon; Y = spacer; R1 = H, (un)substituted hydrocarbon group, (un)substituted cyclic group; R2, R3 = H, (un)substituted hydrocarbon group; (un)substituted cyclic group, etc.; R2 and R3 together with the nitrogen atom to which they bonded may combine to form an optionally substituted heterocycle containing nitrogen.; R4 = H, (un)substituted hydrocarbon group], salts, N-oxide, solvates or prodrugs thereof were prepared For example, reductive amination of 4-(1-azepanyl)-N-[(2R,3S)-2-(azidomethyl)-3-pyrrolidinyl]-2-pyrimidineamine, e.g., prepared from tert-Bu (2R,3S)-3-[(tert-butyldimethylsilyl)oxy]-2-(hydroxymethyl)-1-pyrrolidinecarboxylate in 9 steps, with cyclohexanone followed by Pd/C catalyzed reduction under H2 afforded (2R,3S)-II [R = CH2NH2]. In CXCR4 binding inhibition assays using human stromal cell derived factor 1 (SDF-1), the IC50 value of (2R,3S)-II [R = (CH2)3NH2] was 1.6 nM. Compds. I are claimed useful for the treatment of AIDS, articular rheumatism, etc.

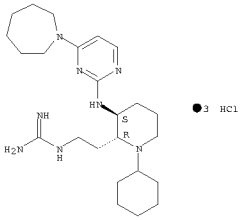
L22 ANSWER 4 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)

IT **908022-00-4P** **908022-01-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-aminopyrimidine compds. as CXCR4 antagonists for treatment of AIDS, articular rheumatism, etc.)

RN 908022-00-4 ZCAPLUS

CN Guanidine, N-[2-[(2R,3S)-1-cyclohexyl-3-[[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]amino]-2-piperidinyl]ethyl]-, hydrochloride (1:3), rel- (CA INDEX NAME)

Relative stereochemistry.

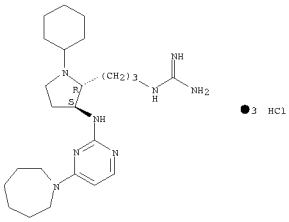


●3 HCl

RN 908022-01-5 ZCAPLUS

CN Guanidine, N-[3-[(2R,3S)-1-cyclohexyl-3-[[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]amino]-2-pyrrolidinyl]propyl]-, hydrochloride (1:3), rel- (CA INDEX NAME)

Relative stereochemistry.



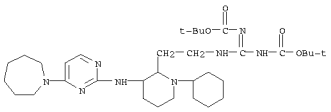
●3 HCl

IT **908128-34-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-aminopyrimidine compds. as CXCR4 antagonists for treatment of AIDS, articular rheumatism, etc.)

RN 908128-34-7 ZCAPLUS

CN Carbamic acid, [[[2-[(2R,3S)-1-cyclohexyl-3-[[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]amino]-2-piperidinyl]ethyl]amino]][(1,1-

L22 ANSWER 4 OF 4 ZCAPLUS COPYRIGHT 2011 ACS on STN (Continued)
dimethylethoxy)carbonyl]amino]methylene]-, 1,1-dimethylethyl ester, [N(E)]-rel- (9CI) (CA INDEX NAME)



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L1             1 US20060217379 /PN

     FILE 'REGISTRY' ENTERED AT 14:08:39 ON 11 JAN 2011

     FILE 'ZCAPLUS' ENTERED AT 14:08:39 ON 11 JAN 2011
L2             TRA L1 1- RN :      389 TERMS

     FILE 'REGISTRY' ENTERED AT 14:08:39 ON 11 JAN 2011
L3           389 SEA L2
L4           336 NCNC3/ES AND L3
L5               STR
L6       1749673 46.195/RID AND NRS>=3
L7            50 L5 SAM SUB=L6
L8               STR L5
L9            50 L8 SAM SUB=L6
L10              STR L8
L11            0 L10 SAM SUB=L6
L12              STR L5
L13            0 L12 SAM SUB=L6
L14        26410 L5 FULL SUB=L6
                 SAV TEM J657C1/A L14
L15            0 L12 SAM SUB=L14
L16              STR L12
L17            0 L16 SAM SUB=L14
L18           16 L16 FULL SUB=L14
                 SAV TEM J657C1N/A L18
L19            0 L18 AND L3
L20          113 L3 AND N>=6
L21          112 L20 AND L4

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L22            4 L18

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